

REPORT 1283

EXTRAPOLATION TECHNIQUES APPLIED TO MATRIX METHODS IN NEUTRON DIFFUSION PROBLEMS¹

By ROBERT R. MCCREADY

SUMMARY

A general matrix method is developed for the solution of characteristic-value problems of the type arising in many physical applications. The scheme employed is essentially that of Gauss and Seidel with appropriate modifications needed to make it applicable to characteristic-value problems. An iterative procedure produces a sequence of estimates to the answer; and extrapolation techniques, based upon previous behavior of iterants, are utilized in speeding convergence. Theoretically sound limits are placed on the magnitude of the extrapolation that may be tolerated.

This matrix method is applied to the problem of finding criticality and neutron fluxes in a nuclear reactor with control rods. The two-dimensional finite-difference approximation to the two-group neutron-diffusion equations is treated. Results for this example are indicated.

The calculations were performed on the IBM card-programmed calculator.

INTRODUCTION

A general matrix method is developed for the solution of characteristic-value problems of a type arising in many physical applications. The method of this paper is essentially that of Gauss and Seidel (ref. 1), which itself is but a special case of the method of conjugate gradients (ref. 2). The adaptation of the Gauss-Seidel technique to the characteristic-value problem calls for a means of computing successive estimates of the characteristic value as well as the vector. This calculation is made to rely upon Turner's technique (ref. 3) for assigning a meaning to the ratio of two vectors.

Extrapolation techniques are also employed to speed up the convergence of the iterative process. One of these is based on Turner's original formula (ref. 3), and the other is a slightly more complicated modification.

The number of iterations required for convergence is not studied theoretically here as in the "n-step" methods, but the minimization of a suitable form at each step is derived.

The method is applied to two-group neutron-diffusion equations. The calculations were performed at the NACA Lewis laboratory.

SYMBOLS

The following symbols are used in this report:

A, B, L, U	matrices
B_z^2	axial leakage
D, E, F, G, J, X	vectors
h	grid dimension
i, j, k	indices
k_{th}	thermal multiplication constant
L_f^2	average square slowing down length for fast neutrons
L_{th}^2	average square diffusion length for thermal neutrons
N	number of nuclei per cc
p_{th}	resonance escape probability
r	radial coordinate
r_c	core radius
$\operatorname{sgn} u =$	$\begin{cases} 1 & u > 0 \\ -1 & u < 0 \\ 0 & u = 0 \end{cases}$
t	reflector thickness
w, ω	weight functions
γ	characteristic value
$\Delta_{k+1}^{(i)}$	deviation at i th point of k th iteration (eq. (80))
$\delta_{k+1}^{(i)}$	difference $X_{k+1}^{(i)} - X_k^{(i)}$
λ	actual damping rate
τ	bulk damping rate
$\varphi, \psi, \varphi_{th}, \varphi_f$	neutron fluxes

Parameter groupings:

$$\begin{aligned}
 a &= \frac{1}{L_{f0}^2} + B_z^2 & a' &= \frac{1}{L_{f0}^2} \\
 b &= \frac{\lambda_{tr, th0}}{\lambda_{tr, f0}} k_{th0} \frac{1}{L_{th0}^2} \\
 c &= \frac{1}{L_{th0}^2} + B_z^2 & c' &= \frac{1}{L_{th0}^2} \\
 \bar{d} &= \frac{\lambda_{tr, f0}}{\lambda_{tr, th0}} p_{th0} \frac{1}{L_{f0}^2} \\
 f &= \frac{1}{L_{f1}^2} + B_z^2 & f' &= \frac{1}{L_{f1}^2}
 \end{aligned}$$

¹ Supersedes NACA TN 3511, "Extrapolation Techniques Applied to Matrix Methods in Neutron Diffusion Problems," by Robert R. McCready, 1955.

$$g = \frac{1}{L_{ih_1}^2} + B_z^2 \quad g' = \frac{1}{L_{ih_1}^2}$$

$$m = \frac{\lambda_{tr, f_1}}{\lambda_{tr, th_1}} p_{th_1} \frac{1}{L_{f_1}^2}$$

Subscripts:

<i>f</i>	fast
<i>th</i>	thermal
<i>tr</i>	transport
0	reactor
1	reflector
2	rod

THE METHOD

MATRIX FORMULATION

Consider the matrix equation

$$AX = \gamma BX \quad (1)$$

where A and B are $n \times n$ matrices, X is an n -component vector, and the characteristic value of γ is a scalar to be determined. A may be separated into the sum of two triangular matrices L and U , where L contains all the diagonal elements of the original matrix A .

This separation, which anticipates the Gauss-Seidel process, is effected in the following manner:

$$A = L + U \quad (2)$$

$$l_{ij} = a_{ij} \quad j \leq i; \quad l_{ij} = 0 \quad j > i \quad (3)$$

$$u_{ij} = a_{ij} \quad j > i; \quad u_{ij} = 0 \quad j \leq i \quad (4)$$

If L is a nonsingular matrix (always true if $l_{ii} \neq 0$ for all i), equation (1), modified to

$$(L + U)X = \gamma BX \quad (5)$$

may be multiplied by L^{-1} , giving

$$(I + L^{-1}U)X = \gamma L^{-1}BX \quad (6)$$

For a given X , the quantities $L^{-1}UX$ and $L^{-1}BX$ of equation (6) may be calculated without the actual formation of L^{-1} . This fact, which is very helpful for systems containing matrices, arises in the following manner and depends upon the triangular nature of L . Let D be the vector defined by

$$D = L^{-1}UX \quad (7)$$

Then

$$LD = UX = C \quad (8)$$

whence

$$l_{11}d_1 = c_1 \quad (9)$$

gives d_1 , since all the c_i can be computed from U and X in equation (8). Then

$$l_{21}d_1 + l_{22}d_2 = c_2 \quad (10)$$

gives d_2 , and

$$l_{31}d_1 + l_{32}d_2 + l_{33}d_3 = c_3 \quad (11)$$

gives d_3 , and so forth, so that L^{-1} need not be computed in order to obtain $L^{-1}UX$. The same argument applies to $L^{-1}BX$.

ITERATIVE SCHEME

Equation (6) may be written

$$X = \gamma L^{-1}BX - L^{-1}UX \quad (12)$$

which may be interpreted as defining the iterative scheme

$$X_{k+1} = \gamma_{k+1} L^{-1}BX_k - L^{-1}UX_k \quad (13)$$

in which γ_{k+1} is an estimate to γ that can be calculated from X_k . To obtain γ_{k+1} , form the inner product of the vector $\text{sgn } L^{-1}BX_k$ with each side of equation (6); thus,

$$\gamma_{k+1} = \frac{(\text{sgn } L^{-1}BX_k, (I + L^{-1}U)X_k)}{(\text{sgn } L^{-1}BX_k, L^{-1}BX_k)} \quad (14)$$

Equations (13) and (14) are the basic equations of the iterative scheme. Given any X_k , γ_{k+1} is computed from equation (14) and γ_{k+1} and X_k are placed in (13) to yield the next iterant X_{k+1} . This process is repeated until X_k and γ_{k+1} converge.

Some normalization is necessary in problems of a homogeneous nature. The simplest method of normalization is to adjust a permanently specified coordinate of X_k to unity before beginning each iteration. This is accomplished by dividing each element of the vector by the specified coordinate.

The ratio defined by equation (14) was chosen for simplicity of calculation on available punched-card equipment. That ratio can be compared to the Rayleigh quotient (for eq. (13))

$$\gamma'_{k+1} = \frac{(J_k, G_k)}{(J_k, J_k)} \quad (15)$$

where

$$J_k = L^{-1}BX_k \quad (16)$$

$$G_k = (I + L^{-1}U)X_k \quad (17)$$

by noting that each of the relations (14) and (15) constitutes a weighted sum of local (point by point) values $\gamma_{k+1}^{(i)}$ of γ'_{k+1} . These local values are defined by

$$\gamma_{k+1}^{(i)} = \gamma_{k+1}^{(i)} = g_k^{(i)} / j_k^{(i)} \quad (18)$$

where $g_k^{(i)}$ and $j_k^{(i)}$ are the i th components of G_k and J_k , respectively. The weighted average associated with (15) is

$$\gamma'_{k+1} = \sum_i w_i \gamma_{k+1}^{(i)} \quad (19)$$

where

$$w_i = \frac{[j_k^{(i)}]^2}{\sum_m [j_k^{(m)}]^2} \quad (20)$$

while the weighted average associated with (14) is

$$\gamma_{k+1} = \sum_i \omega_i \gamma_{k+1}^{(i)} \quad (21)$$

where

$$\omega_i = \frac{|j_k^{(i)}|}{\sum_m |j_k^{(m)}|} \quad (22)$$

Equation (15) selects that value of γ'_{k+1} which minimizes the sum of the squares of the residuals of equation (6) when that quantity is thought of as a function of γ'_{k+1} . The sum

of the squares of the residuals is not, of course, the only quadratic form that is suitable for minimization (ref. 2). Consider the expression

$$p = p(\gamma_{k+1}) = \sum_i \left\{ \frac{g_k^{(i)} \operatorname{sgn} j_k^{(i)}}{[j_k^{(i)} \operatorname{sgn} j_k^{(i)}]^{1/2}} - \gamma_{k+1} [j_k^{(i)} \operatorname{sgn} j_k^{(i)}]^{1/2} \right\}^2 \quad (23)$$

which is zero for $X_k = X$ and $\gamma_{k+1} = \gamma$. This generally positive quantity can be minimized (made closer to its ultimate value zero) by setting

$$\gamma_{k+1} = \frac{(\operatorname{sgn} J_k, G_k)}{(\operatorname{sgn} J_k, J_k)} \quad (24)$$

which is equation (14) expressed in terms of J and G .

EXAMPLE

To illustrate the convergence of this method in a special case, consider the problem of equation (1) with

$$A = \begin{pmatrix} 3 & -1 & -1 & 0 \\ 0 & 2 & -1 & -1 \\ 0 & -1 & 3 & -1 \\ 0 & -1 & -2 & 3 \end{pmatrix} \quad (25)$$

and

$$B = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad (26)$$

which has the real solution $X^{(1)} = 1.020070$, $X^{(2)} = 1.329658$, $X^{(3)} = 1.000000$, $X^{(4)} = 1.109886$; $\gamma = 0.549429$ and two solutions with complex characteristic values. This solution was found by the ordinary process of solving the characteristic equation.

This problem was solved in 15 iterations starting with an initial guess of $X_0 = (10, 100, 1, 1000)$. The values of successive iterants, together with those of γ , are listed in the following table. The iterants are normalized so that $X_k^{(3)} = 1$ at the start of each iteration:

k	$X_k^{(1)}$	$X_k^{(2)}$	$X_k^{(4)}$	γ_{k+1}
0	10	100	1000	
1	-0.692996	1.069635	1.023212	-10.034589
2	.271412	.488315	.812771	-1.352353
3	.848870	1.565152	1.188394	-.097105
4	1.132470	1.360721	1.120240	.526554
5	1.006120	1.292707	1.097568	.592807
6	1.010639	1.337044	1.112348	.538366
7	1.024544	1.331918	1.110639	.547271
8	1.018872	1.328104	1.109363	.551383
9	1.019593	1.328348	1.109949	.549107
10	1.020236	1.329788	1.109929	.549291
11	1.020078	1.329596	1.109865	.549510
12	1.020048	1.329600	1.109886	.549423
13	1.020076	1.329665	1.109889	.549422
14	1.020071	1.329656	1.109885	.549432
15	1.020070	1.329658	1.109886	.549430

EXTRAPOLATION TECHNIQUE

If, instead of four components, the iterant vector has many components, techniques of extrapolation are usually desirable to speed convergence of the process. The technique employed here, which is due to Turner (ref. 3), attempts to

evaluate a bulk damping rate that describes in an average way the over-all trend of the individual components of the iterant vectors.

Assume that each iterant X_k is made up of the sum of the solution X and two error vectors E_k and F_k satisfying the damping relations

$$E_{k+1} + \tau E_k \quad (27)$$

and

$$F_{k+1} = -\tau F_k \quad (28)$$

Then the following relations hold:

$$X_0 = X + E_0 + F_0 \quad (29)$$

$$X_1 = X + \tau E_0 - \tau F_0 \quad (30)$$

$$X_2 = X + \tau^2 E_0 + \tau^2 F_0 \quad (31)$$

$$X_3 = X + \tau^3 E_0 - \tau^3 F_0 \quad (32)$$

One may compute

$$\tau^2 = \frac{X_3 - X_2}{X_1 - X_0} \quad (33)$$

The "vector division" implied in equation (33) is possible because, under the initial assumption of error behavior (eqs. (27) and (28)), the vectors $X_3 - X_2$ and $X_1 - X_0$ are collinear and therefore differ only in length.

If the error vectors are eliminated from equations (30) and (32), one obtains

$$X = \frac{X_3 - \tau^2 X_1}{1 - \tau^2} \quad (34)$$

which gives the answer as a linear combination of the alternate iterants X_1 and X_3 .

The preceding analysis suggests that a formula analogous to (34) be used to estimate the answer. The difficulty here is that equation (33) may be meaningless when equations (29) to (32) do not hold. To circumvent this difficulty, a method of computing τ^2 is needed. Toward this end, define δ_{k+1}^{ϕ} by means of

$$\delta_{k+1}^{\phi} = X_{k+1}^{\phi} - X_k^{\phi} \quad (35)$$

and define τ^2 by means of

$$\tau^2 = \frac{\sum_j \delta_j^{\phi} \operatorname{sgn} \delta_1^{\phi}}{\sum_j |\delta_j^{\phi}|} \quad (36)$$

The direct analogy to equation (14) will be noticed. Equation (36) permits computation, in an average way, of the damping of the error vectors. With τ^2 available, the extrapolated value X' of X is computed from

$$X' = \frac{X_3 - \tau^2 X_1}{1 - \tau^2} \quad (37)$$

In case the error is damping exactly as assumed in (27) and (28), equation (36) gives the value indicated by (33), and equation (37) reduces to (34); that is, X' becomes the answer X .

Since the ideal damping behavior is rarely an actuality, it is of interest to examine the effect of the preceding process on

error components. Suppose that X_0 is more adequately represented by

$$X_0 = X + \sum_{i=1}^n E_0^{(i)} \quad (38)$$

where $E_0^{(i)}$ has a damping rate (positive or negative) of λ_i . Then

$$X_3 = X + \sum_{i=1}^n \lambda_i^3 E_0^{(i)} \quad (39)$$

and

$$X_1 = X + \sum_{i=1}^n \lambda_i E_0^{(i)} \quad (40)$$

hold. The extrapolation indicated in equation (37) now yields the following relation between the estimate X' and the answer X :

$$X' = X + \sum_{i=1}^n \frac{\lambda_i(\lambda_i^2 - \tau^2)}{1 - \tau^2} E_0^{(i)} \quad (41)$$

This interpretation is useful, since it indicates the damping effect upon the errors of three iterations and one extrapolation.

If, for simplicity, one of the errors $E_0^{(i)}$ and its damping rate λ_i are designated by E and λ , respectively, then

$$R(\lambda, \tau) = \frac{(\lambda^2 - \tau^2)\lambda^{j-2}}{1 - \tau^2} \quad (42)$$

gives the damping of this error component as a result of j iterations and one extrapolation. The "extreme" value of R (actually that value farthest from zero; i. e., farthest from maximum damping) may be found by setting

$$\frac{dR}{d\lambda} = \frac{j\lambda^{j-1} - \tau^2(j-2)\lambda^{j-3}}{1 - \tau^2} = 0 \quad (43)$$

This yields

$$\lambda^2 = \left(\frac{j-2}{j}\right) \tau^2 \quad (44)$$

as the equation to be solved for the values of λ which are associated with the errors that receive the minimum damping from the process of j iterations and one extrapolation. Equations (42) and (44) give $R_{ext}(\tau)$, the extreme value of R , as a function only of τ and j :

$$R_{ext}(\tau) = \frac{-2\tau^j}{1 - \tau^2} \frac{1}{j-2} \left(\frac{j-2}{j}\right)^{j/2} \quad (45)$$

To find the value of τ^2 so that this function (R_{ext}) cannot exceed the bounds ± 1 [i. e., so that the slowest damping component (and hence all components) cannot increase through extrapolation], τ must be less in absolute value than the least of the roots of

$$\pm \left(\frac{2}{j-2}\right) \left(\frac{j-2}{j}\right)^{j/2} \tau^j - \tau^2 + 1 = 0 \quad (46)$$

If only such τ^2 are used, the convergence of the process cannot be impaired by the extrapolation.

Suppose now that the previous value of $R(\lambda, \tau)$ is replaced by the formula

$$\tilde{R}(\lambda, \tau) = \frac{\lambda^{j-4}(\lambda^2 - \tau^2)}{1 - \tau^2} \frac{\lambda^2 - \frac{j-2}{j} \tau^2}{1 - \frac{j-2}{j} \tau^2} \quad (47)$$

In formula (47), $j \geq 4$. The second factor places a zero (maximum damping) at just the points of minimum damping, that is, at the values of λ determined by (44). If now $d\tilde{R}/d\lambda$ is taken as zero and the limit ± 1 is placed upon the resulting $R_{ext}(\tau^2)$, the limiting safe values of τ^2 are obtained by finding the least of the roots of

$$[j\tau^j - 2(j-1)\tau^{j-2} + (j-2)\tau^{j-4}] \tau^j \pm [j-2(j-1)\tau^2 + (j-4)\tau^4] = 0 \quad (48)$$

where τ^2 satisfies

$$\tau^2 = \frac{(j-1)(j-2) \pm \sqrt{5j^2 - 12j + 4}}{j^2} \quad (49)$$

The revised formula (47) has both the effect of ensuring that no component will be impaired in its damping by the extrapolation and also that the least rapidly damping component receives a zero contribution in the extrapolation.

Since, as before, for some error component E ,

$$X_j = X + \lambda^j E \quad (50)$$

$$X_{j-2} = X + \lambda^{j-2} E \quad (51)$$

$$X_{j-4} = X + \lambda^{j-4} E \quad (52)$$

in which X represents the answer, the specification of (47) as a damping formula implies

$$X' = X + \frac{j\lambda^j - 2(j-1)\tau^2\lambda^{j-2} + (j-2)\tau^4\lambda^{j-4}}{j-2(j-1)\tau^2 + (j-2)\tau^4} E \quad (53)$$

where X' is the extrapolated value of X_j . If $\lambda^j E$, $\lambda^{j-2} E$, and $\lambda^{j-4} E$ are eliminated from (53) using the relations (50), (51), and (52), then

$$X' = \frac{jX_j - 2(j-1)\tau^2 X_{j-2} + (j-2)\tau^4 X_{j-4}}{j-2(j-1)\tau^2 + (j-2)\tau^4} \quad (54)$$

Comparison of (42) (with $j=3$) with (37) on one hand and of (47) with (54) on the other hand leads to the following valid rule of thumb to obtain the extrapolated value of X for a given damping function: Replace the power λ^j of λ in the damping function by X_j ; the resulting linear combination of alternate iterants is the formula for the extrapolated X . It is easily verified that the validity of this arises from the manner in which the error vectors are assumed to behave.

The smallest roots of equations (46) and (48) are listed in the following tables:

Eq. (46)		Eq. (48)	
j	τ^2	j	τ^2
4	0.8284	4	0.6667
6	.8941	6	.8745
8	.9233	8	.9213
10	.9399	10	.9427

These are the upper limits of the "safe" values of τ^2 within the framework of the definition.

APPLICATION TO REACTOR THEORY

GENERAL REMARKS

Multigroup reactor equations can be solved, in principle, by the present method. The number of components in the vector solution, to be discussed in detail later, is approximately equal to the product of the number of grid points and the number of groups in the multigroup scheme. An extreme increase in the number of these elements lengthens the problem considerably. The calculations here are performed in accordance with two-group neutron-diffusion theory.

The two-dimensional reactor with control rods, which is considered later, is suited to two-group calculations, since the control rods are particularly effective on the thermal group, and two-group calculations are good for thermal assemblies.

The following illustration is introduced to show the general principles of the matrix setup in detail. These principles do not change for the more complicated two-dimensional problem that is treated later. A relatively simple one-dimensional problem has been chosen to illustrate the detailed setup and the consequent matrix.

EXAMPLE OF TWO-GROUP DIFFUSION EQUATIONS

The one-dimensional diffusion equations for a reflected thermal reactor of slab geometry are (ref. 4)

$$\frac{d^2\varphi_f}{dr^2} - a'\varphi_f = -\gamma b\varphi_{in} \quad (55)$$

and

$$\frac{d^2\varphi_{in}}{dx^2}-c'\varphi_{in}+\bar{d}\varphi_f=0 \quad (56)$$

for the core, and

$$\frac{d^2\varphi_f}{dx^2} - f'\varphi_f = 0 \quad (57)$$

and

$$\frac{d^2\varphi_{in}}{dx^2}-g'\varphi_{in}+m\varphi_f=0 \quad (58)$$

for the reflector.

The parameters a' , b , c' , \bar{d} , f' , g' , and m are defined in the list of symbols; γ is the characteristic value of the system and equals 1 for criticality. When γ converges to a value other than unity, the uranium concentration is adjusted and the process repeated.

The differential equations (55) to (58) are replaced by finite-difference equations; the operation $d^2\varphi/dx^2$ is estimated by means of the approximate formula

$$h^2 \frac{d^2 \varphi}{dx^2} \Big|_{x=x_i} = \varphi_{i+1} + \varphi_{i-1} - 2\varphi_i \quad (59)$$

where the points of the region are numbered in order as grid points of a finite-difference net, and h is the distance between successive points. In the following, r_c is the core radius, r_{c+i} the complete reactor radius, and point 6 lies on the interface:

$$\begin{array}{cccccccccc}
. & & & & & & . & & . & \\
. & & 0 & & & & . & 1 & . & \\
. & & & & & & . & & . & \\
. & & & & & & . & & . & \\
0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 \\
0 & & & & & & r_c & & r_{c+1} &
\end{array}$$

The boundary conditions are that the fast and thermal fluxes have zero current across the plane of symmetry ($x=0$). This condition

$$-\lambda_{ir} \frac{d\varphi}{dx} \Big|_{x=0} = 0 \quad (60)$$

can be approximated by

$$\frac{\varphi_1 - \varphi_0}{h} = 0 \quad (60a)$$

for both φ_f and φ_{th} . The condition of continuity of currents at the interface is met by approximating the derivatives in the expression

$$-\lambda_{i\tau_0} \frac{d\varphi}{dx}(r_c-0) = -\lambda_{i\tau_1} \frac{d\varphi}{dx}(r_c+0) \quad (61)$$

for both the fast and thermal fluxes. The remaining condition is that the flux be zero at the outer boundary. If the fast flux is designated by φ and the thermal by ψ , the system becomes:

Equation

$$\left. \begin{aligned} j & \\ 0 & \quad \frac{\varphi_1 - \varphi_0}{h} = 0 \\ 1-5 & \quad \frac{\varphi_{j+1} + \varphi_{j-1} - 2\varphi_j}{h^2} - a' \varphi_j = -\gamma b \Psi_j \\ 6 & \quad \gamma_{ir,r0} \frac{\varphi_8 - \varphi_5}{h} = \lambda_{ir,r1} \frac{\varphi_7 - \varphi_6}{h} \\ 7 & \quad \frac{\varphi_8 + \varphi_5 - 2\varphi_7}{h^2} - f' \varphi_7 = 0 \\ 8 & \quad \frac{\varphi_7 - 2\varphi_8}{h^2} \Big|_{n=1}^1 + f' \varphi_8 = 0 \text{ which incorporates } \varphi_9 = 0 \end{aligned} \right\} \quad (62)$$

for the fast-balance equations and, for the thermals:

Equation

$$\left. \begin{aligned} &0 \quad \psi_1 - \psi_0 = 0 \\ &1-5 \quad \frac{\psi_{i+1} + \psi_{i-1} - 2\psi_i}{\hbar^2} - c' \psi_i + \bar{d} \varphi_i = 0 \\ &6 \quad \lambda_{ir, i\hbar^0} \frac{\psi_6 - \psi_5}{\hbar} = \lambda_{ir, i\hbar^1} \frac{\psi_7 - \psi_6}{\hbar} \\ &7 \quad \frac{\psi_8 + \psi_6 - 2\psi_7}{\hbar^2} - g' \psi_7 + m \varphi_7 = 0 \\ &8 \quad \frac{\psi_7 - 2\psi_8}{\hbar^2} - g' \psi_8 + m \varphi_8 = 0 \text{ which incorporates } \psi_9 = 0 \end{aligned} \right\} \quad (63)$$

The variables φ_0 to φ_8 and ψ_0 to ψ_8 may now be written as X_0 to X_8 and X_9 to X_{17} , respectively. The matrix formulation of these equations is presented in figure 1. The following symbols have been introduced:

$$I_h = 1/h^2 \quad (64)$$

$$A_h = 2/h^2 + a \quad (65)$$

$$F_h = 2/h^2 + f \quad (66)$$

$$C_h = 2/h^2 + c \quad (67)$$

$$G_h = 2/h^2 + g \quad (68)$$

$$L = \frac{\lambda_{tr, r0}}{\lambda_{tr, r1}} \quad (69)$$

$$S = \frac{\lambda_{tr, r0}}{\lambda_{tr, r1}} \quad (70)$$

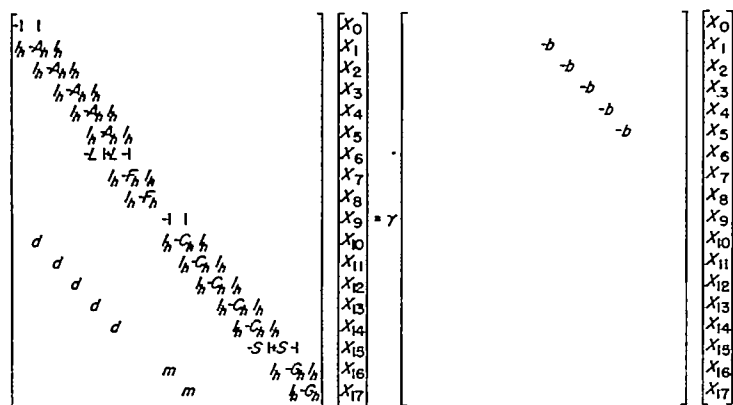


FIGURE 1.—Matrix formulation of equations (62) and (63).

RECAPITULATION

To review the general application of the method to two-group reactor equations, consider the following broad outline of this process:

(1) Write the two-group equations with the parameter γ introduced as a multiplier of the production term of the fast-balance equations.

(2) Express the differential equations by their finite-difference approximations so that they become a linear algebraic set of the type associated with equation (1).

(3) Perform such iterations and extrapolations as necessary to obtain well-converged values of γ and X .

(4) Adjust the uranium concentration and repeat step (3) using the original answer from (3) for the initial guess X_0 . The concentration should be changed so that $\gamma \rightarrow 1$.

(5) Repeat (3) and (4) until γ converges. If criticality is desired, change the concentration so that the converged values of $\gamma \rightarrow 1$.

TWO-DIMENSIONAL REACTOR WITH CONTROL RODS

GEOMETRY OF REACTOR

The reactor (see fig. 2) is cylindrical and water-reflected with a core composed of aluminum, water, and uranium, which are assumed to be homogeneously mixed. The height of the reactor is 70 centimeters, the outside radius 50 centimeters, and the core radius 32 centimeters. Nine

cadmium control rods are inserted in the core; one, a cylindrical rod of 2-centimeter radius, is centered along the axis of the reactor. The remaining eight rods are equally spaced on a radius of 24 centimeters and are shaped so as to be bounded by coordinate surfaces. Each of these rods extends over a radial distance of 4 centimeters and subtends a central angle of 9° .

The symmetry of this assembly is an important factor in making solution of the reactor problem feasible. The flux in the 45° sector indicated in figure 2 is adequate to represent the flux in the entire reactor; in fact, additional symmetry within the sector implies that only half the sector need be considered. The three-dimensional problem is made two-dimensional (computation-wise) by estimating the neutron leakage in the axial direction due to the finite height of the reactor. This is based upon an axial cosine distribution similar to the bare pile solution (eq. (75)).

COMPOSITION AND NUCLEAR PARAMETERS

The core volume is proportioned between the water (density, 1 g/cc) and aluminum by assuming a volume ratio of aluminum to water of 0.76. The nuclear diffusion constants for the core and reflector are listed in the following tables. The subscripts 0, 1, and 2 refer to the core, reflector, and rod regions of the reactor, respectively:

Fast		
Zone	L_f^2	λ_f
0	64	3.78
1	33	3.43
2	----	4.35

Thermal				
Zone	L_{th}^2	λ_{th}	ρ_{th}	k_{th}
0	3.471	0.815	0.95	1.675
1	8.3	.43	.98	-----

Parameters for the rod regions are unnecessary because of the simplified treatment of the rod, in which the thermal neutron flux is assumed to vanish on the rod boundary and the radial and axial leakages are assumed to balance in the absence of fast-neutron absorption processes. The thermal parameters in the preceding table are those associated with an atom ratio of N^H/N^u of 350; these, of course, change for different uranium concentrations.

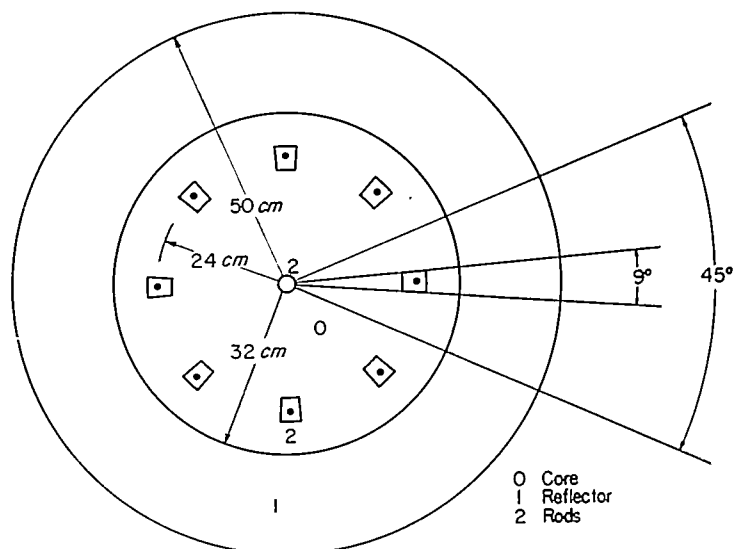


FIGURE 2.—Two-dimensional reactor.

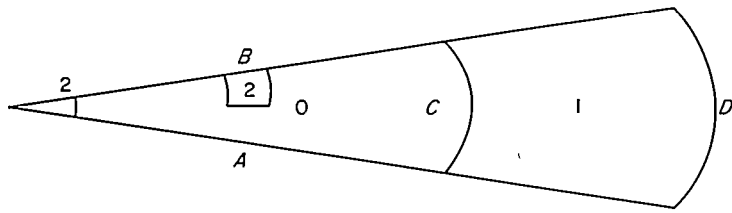


FIGURE 3.—22½° Sector of reactor.

EQUATIONS AND BOUNDARY CONDITIONS

The two-group equations (ref. 4) for the core are taken to be

$$\nabla^2 \varphi_{f0} - \left(\frac{1}{L_{f0}^2} + B_z^2 \right) \varphi_{f0} = -\gamma \frac{\lambda_{tr, f0}}{\lambda_{tr, f0}} k_{f0} \frac{1}{L_{f0}^2} \varphi_{th0} \quad (71)$$

and

$$\nabla^2 \varphi_{th0} - \left(\frac{1}{L_{th0}^2} + B_z^2 \right) \varphi_{th0} + \frac{\lambda_{tr, f0}}{\lambda_{tr, th0}} p_{th0} \frac{1}{L_{f0}^2} \varphi_{f0} = 0 \quad (72)$$

All the parameters of equations (71) and (72) are the ordinary nuclear ones, except the arbitrarily inserted γ , which is a measure of the criticality and is equal to 1 for a critical assembly.

In the reflector the two-group diffusion equations take the form

$$\nabla^2 \varphi_{f1} - \left(\frac{1}{L_{f1}^2} + B_z^2 \right) \varphi_{f1} = 0 \quad (73)$$

$$\nabla^2 \varphi_{th1} - \left(\frac{1}{L_{th1}^2} + B_z^2 \right) \varphi_{th1} + \frac{\lambda_{tr, f1}}{\lambda_{tr, th1}} p_{th1} \frac{1}{L_{f1}^2} \varphi_{f1} = 0 \quad (74)$$

while the fast-diffusion equation for the rods is taken to be

$$\nabla^2 \varphi_{f2} - B_z^2 \varphi_{f2} = 0 \quad (75)$$

Any change in rod boundary conditions would not affect the general principles of the numerical scheme. As will be seen from the boundary conditions, the thermal neutrons do not require a diffusion equation within the rods. The region considered in the problem is a 22½° sector (of the circle of fig. 2), one side of which passes through the center of one of the outlying rods. This is illustrated in figure 3. The symmetry of the over-all reactor implies that the normal derivatives of the flux across the surfaces *A* and *B* are zero. This implies that the flux at all points of the circle of figure 2 can be found by solution for the flux only in the sector indicated in figure 3. The condition of continuity of fluxes and currents is involved at the core-reflector interface, indicated by *C* in figure 3. The vanishing of the fast and thermal flux at the outer boundary (*D*) is also required. The thermal flux is taken as zero on the edge of the control rod, and the continuity of the fast flux and current is considered to hold on the core-rod interfaces. The details of the mathematical formulation of these conditions are deferred until the general discussion of the difference equations.

FINITE-DIFFERENCE EQUATIONS

In order to write the reactor equations as finite-difference approximations, the sector of figure 3 is divided into a grid net of points. The flux is determined by solution of the

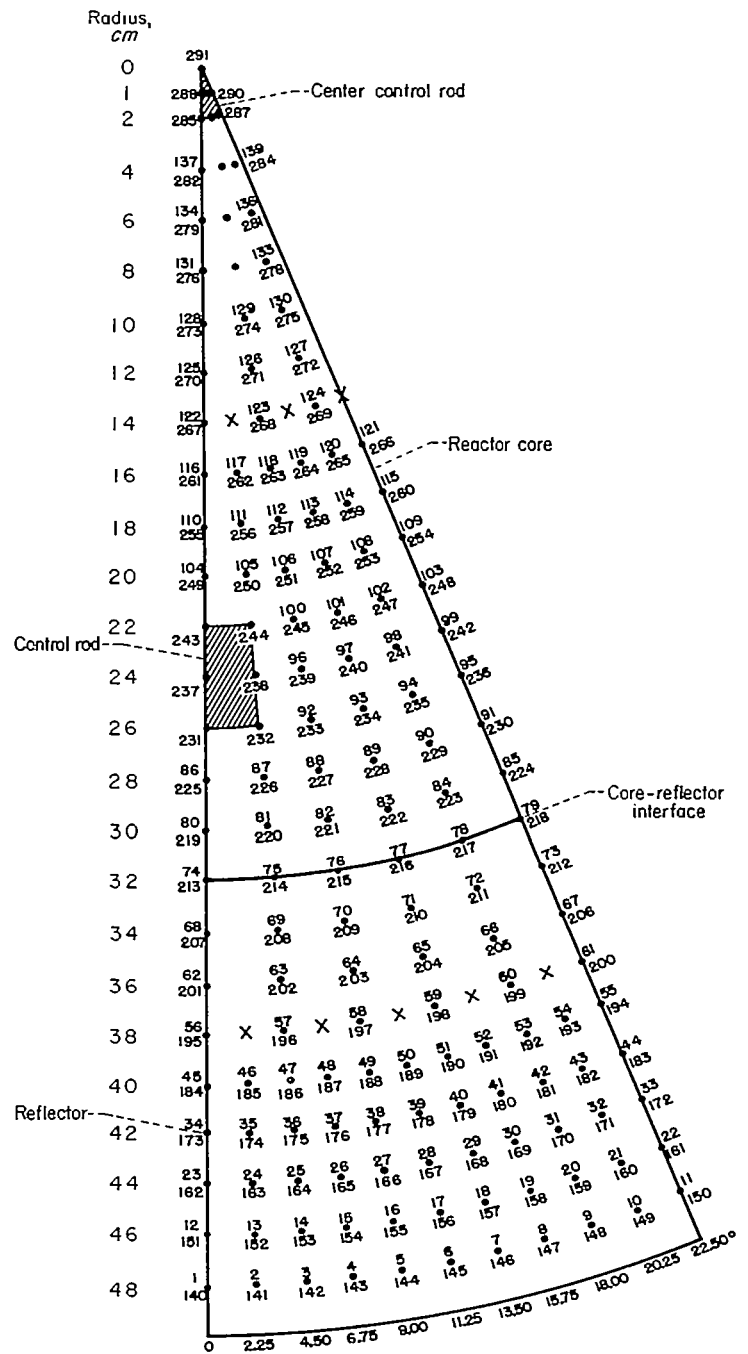


FIGURE 4.—Reactor grid points.

linear algebraic system of equations that results from writing the finite-difference approximation to the fast- and thermal-diffusion equations at each point. The grid arrangement used in the present problems is indicated in figure 4. The thermal flux (components 1 to 139 of the vector solution) has the following breakdown into groups of components: reflector (1 to 73), core-reflector interface (74 to 79), core (80 to 139). The fast flux (140 to 291) has the following breakdown: reflector (140 to 212), core-reflector interface (213 to 218), core (219 to 284), control rods (231, 232, 237, 238, 243, 244, and 285 to 291).

The number of components associated with the thermal and fast fluxes, respectively, differs because of the assignment of boundary conditions at the control rods, which brings the fast flux into a larger area of definition.

For two-dimensional cylindrical geometry, the operation of the form $\nabla^2 \varphi$ is given by

$$\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} + \frac{\partial^2}{\partial \theta^2} \quad (76)$$

This form is to be replaced by a difference operation that relates each point to its four nearest neighbors. If the point in question is designated by the subscript zero and the others are

$$\begin{array}{c} 1 \\ \cdot \\ h_r \\ 4 \cdot h_\theta \cdot 0 \cdot h_\theta \cdot 2 \quad r \uparrow \theta \rightarrow \\ h_r \\ \cdot \\ 3 \end{array}$$

where h_r and h_θ are the grid widths in the r and θ directions, respectively, then at $\varphi = \varphi_0$ the following approximation is used:

$$\nabla^2 \varphi = \left(\frac{1}{h_r^2} + \frac{1}{2rh_r} \right) \varphi_1 + \left(\frac{1}{h_r^2} - \frac{1}{2rh_r} \right) \varphi_3 + \frac{1}{r^2 h_\theta^2} (\varphi_2 + \varphi_4) - \left(\frac{2}{h_r^2} + \frac{2}{h_\theta^2} \right) \varphi_0 \quad (77)$$

With this designation (and barring certain exceptional points to be discussed later), one may move from point to point on the grid and write equations of neutron balance for each of the two neutron groups.

The following equations may be taken as typical illustrations:

Thermal-balance equation 93 (see fig. 4):

$$\left(\frac{1}{h_r^2} + \frac{1}{2rh_r} \right) X_{89} + \left(\frac{1}{h_r^2} - \frac{1}{2rh_r} \right) X_{97} + \frac{1}{r^2 h_\theta^2} (X_{92} + X_{94}) - \left(\frac{2}{h_r^2} + \frac{2}{h_\theta^2} + \frac{1}{L_{i\theta}^2} + B_z^2 \right) X_{93} + \frac{\lambda_{ir, r0}}{\lambda_{ir, i\theta0}} p_{i\theta0} \frac{1}{L_{r0}^2} X_{234} = 0 \quad (78)$$

Fast-balance equation 234:

$$\left(\frac{1}{h_r^2} + \frac{1}{2rh_r} \right) X_{228} + \left(\frac{1}{h_r^2} - \frac{1}{2rh_r} \right) X_{240} + \frac{1}{r^2 h_\theta^2} (X_{233} + X_{235}) - \left(\frac{2}{h_r^2} + \frac{2}{h_\theta^2} + \frac{1}{L_{r0}^2} + B_z^2 \right) X_{234} = -\gamma \frac{\lambda_{ir, i\theta0}}{\lambda_{ir, r0}} k_{i\theta0} \frac{1}{L_{i\theta0}^2} X_{93} \quad (79)$$

In contradistinction to equations (78) and (79), there are certain special equations that hold at the exceptional points referred to earlier. These equations result from one or more of the following conditions:

- (1) Continuity of currents at interfaces
- (2) Zero flux at the outside boundary
- (3) Zero current across planes of symmetry
- (4) Change in grid dimensions

Condition (1) is treated by matching a suitable ratio of normal derivatives from either side of the interface. Each of these derivatives is evaluated by a five-point differentiation formula. Condition (2) is treated by writing the difference approximation to the diffusion equation for points adjacent to the outside boundary with zero replacing the flux at the boundary point.

Condition (3) is accounted for by writing the diffusion equation of a point on the plane assuming the same flux at grid points on either side of the plane. For condition (4) θ -wise interpolation formulas are used to define fluxes at the points marked X on figure 4, and these are utilized where needed, in writing diffusion equations in the finer net. If each equation of the set is written in order and the production terms are isolated as illustrated in equation (71) then the matrix equation constructed from the approximate finite difference may be written in the form of equation (1).

The matrix B is singular, largely consisting of zero elements with an essentially diagonal group of nonzero terms somewhat off the leading diagonal. The matrix A has a substantial number of nonzero elements crowded quite close to the leading diagonal. This latter situation is numerically desirable, as elements far from the leading diagonal tend to slow the convergence of numerical processes.

If criticality is desired, the concentration of fissionable material is adjusted, after γ and X have converged, and a whole new set of calculations is run until a new value for γ is reached. This process may be continued until $\gamma=1$.

The method can also be used to compute reactivity changes; the calculation time is again shortened considerably if flux distributions are not demanded.

SOLUTIONS OF TWO-DIMENSIONAL PROBLEM

The results of the calculations of the supercritical ($\gamma=0.948$) case are shown in figures 5 to 7. Figure 5 gives the fast flux as a function of r for $\theta=0^\circ$, 9° , and 18° . The control rods have no substantial effect on the fast flux. Figure 6 gives the corresponding thermal flux and shows the localized effect of the control rods. Figure 7 presents iso-flux contours of the thermal flux. The 0.19 contour in the reflector and the 0.234 contour in the core represent relative maximums.

COMMENTS ON APPLICATION OF THE METHOD

A number of numerical quantities may be examined in an attempt to evaluate the degree of convergence of a system. One of the most natural of these quantities is the sum of the squares of the residuals. Another may be formed by considering the fact that, as the limit is approached, the ratio

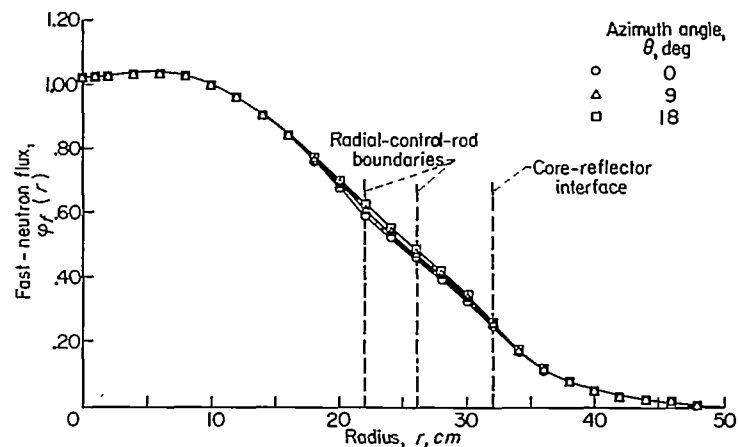


FIGURE 5.—Fast-neutron flux for azimuth angles of 0° , 9° , and 18° .

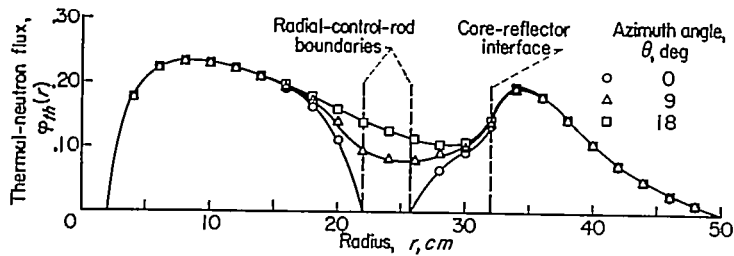


FIGURE 6.—Thermal-neutron flux for azimuth angles of 0°, 9°, and 18°.

$\gamma_{k+1}^{(i)}/\gamma_{k+1}$ must tend toward unity. This means that the deviation defined by

$$\Delta_{k+1}^{(i)} = 1 - \frac{\gamma_{k+1}^{(i)}}{\gamma_{k+1}} \quad (80)$$

must tend toward zero. The average absolute value of the deviation, summed over all points of the reactor, is

$$|\overline{\Delta_{k+1}^{(i)}}| = \frac{\sum_{i=1}^n \left| 1 - \frac{\gamma_{k+1}^{(i)}}{\gamma_{k+1}} \right|}{n} \quad (81)$$

where n is the number of reactor points.

An illustration of the behavior of this quantity is given in the following table:

$k+1$	$ \overline{\Delta_{k+1}^{(i)}} $	$ \Delta_{k+1}^{(i)} _{\max}$
6	0.02199	0.2133
15	.02551	.3156
22	.03254	.0147
31	.00130	.0113
40	.000783	.0051
49	.00028	.0027

The iterants listed are those which just precede the extrapolation process. These are chosen so as to minimize the effect of fluctuations introduced by the extrapolation technique.

These illustrative values come from the second general process; that is, after γ had converged to 1.2064, the concentration (and hence elements of the matrices A and B) was changed and a new series of iterations begun. This converged (more rapidly than the first run) to a value of 0.948.

To estimate the value of uranium concentration needed for the new run, the equation

$$1.2064 k_{th}(\text{old}) = k_{th}(\text{new}) \quad (82)$$

was used to compute a new k_{th} from which to obtain a new concentration. This formula is an approximation, since the influence of a change in concentration upon L_{th}^2 is appreciable. The better rate of convergence of the second run is due to the fact that the flux is relatively independent of the characteristic value, so that the initial estimate for the second run was a relatively good one.

The quantity $|\overline{\Delta_{k+1}^{(i)}}|$ reflects the convergence of γ , which is faster than that of the vector X .

In order to determine the degree of convergence of X , consider the quantities

$$d_{k+1} = \sum_{i=1}^n |\delta_{k+1}^{(i)}| = \sum_{i=1}^n |X_{k+1}^{(i)} - X_k^{(i)}| \quad (83)$$

$$|\overline{\delta_{k+1}^{(i)}}| = \frac{d_{k+1}}{n} \quad (84)$$

and the maximum $|\delta_{k+1}^{(i)}|$ designated by $|\delta_{k+1}^{(i)}|_{\max}$. Typical values of these quantities are as follows:

$\gamma=1.206$				$\gamma=0.948$			
$k+1$	d_{k+1}	$ \overline{\delta_{k+1}^{(i)}} $	$ \delta_{k+1}^{(i)} _{\max}$	$k+1$	d_{k+1}	$ \overline{\delta_{k+1}^{(i)}} $	$ \delta_{k+1}^{(i)} _{\max}$
111	0.0099	0.000034	0.000269	6	0.3299	0.001137	0.00918
122	.0083	.000028	.000176	15	.2139	.000735	.00530
133	.0049	.000017	.000167	22	.0223	.000077	.000204
144	.0028	.000010	.0000904	31	.0044	.000015	.0000668
155	.0023	.000008	.0000709	40	.0020	.000007	.0000245

The sums of the squares of the residuals for the two cases $\gamma=1.206$ and $\gamma=0.948$ are as follows:

$\gamma=1.206$		$\gamma=0.948$	
$k+1$	$\sum R_i^2$	$k+1$	$\sum R_i^2$
111	9.44×10^{-7}	6	1.53×10^{-3}
122	4.98×10^{-7}	15	3.51×10^{-4}
133	2.68×10^{-7}	22	1.80×10^{-5}
144	8.60×10^{-8}	31	1.22×10^{-7}
155	5.37×10^{-8}	40	1.99×10^{-9}

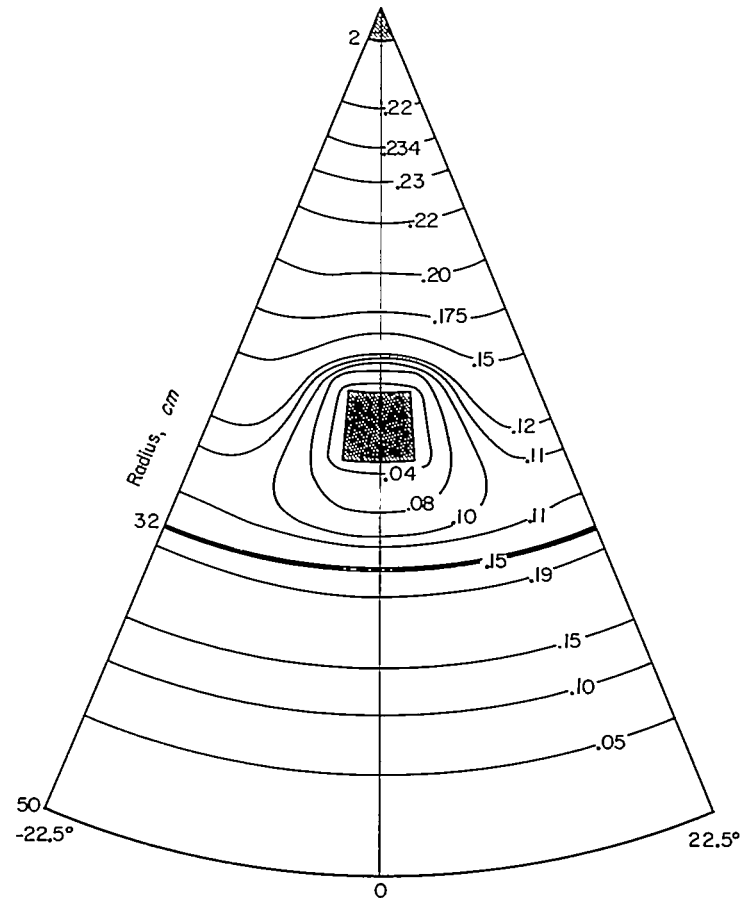


FIGURE 7.—Contour lines for thermal flux.

Several general observations can be made about the process:

(1) The number of iterations in this problem starting from an initial guess to a well-converged value of X was about 150 to 175.

(2) In general, 8 to 10 iterations between extrapolations seem desirable, as the use of too few iterations does not allow the establishment of a fairly uniform damping rate.

(3) The extrapolation formula of equation (37) seems best for rough estimates where error components are being damped rapidly; that of equation (54) seems to be superior for later extrapolations where one is closer to the solution.

(4) When computed values of τ^2 exceed the upper limit, they may be replaced by the limit from the tables giving roots of equations (46) and (48) and then the extrapolation may be carried out, or two more iterations performed with τ^2 recomputed until it falls within prescribed limits.

The following table gives the sum of the squares of the residuals for (a) direct iteration from X_{31} to X_{49} , (b) eight iterations from X_{31} followed by extrapolation with " τ^2 safe" when " τ^2 computed" was too large, then iteration to X_{49} , (c) eight iterations from X_{31} followed by two iterations and

a test until " τ^2 computed" was less than " τ^2 safe," then extrapolation followed by iteration to X_{49} :

Case	ΣR_i^2
(a)	1.35×10^{-7}
(b)	3.44×10^{-9}
(c)	1.68×10^{-4}

LEWIS FLIGHT PROPULSION LABORATORY

NATIONAL ADVISORY COMMITTEE FOR AERONAUTICS

CLEVELAND, OHIO, May 12, 1955

REFERENCES

1. Whittaker, E. T., and Robinson, G.: The Calculus of Observations. Fourth ed., Blackie and Son (London), 1949.
2. Hestenes, Magnus R., and Stiefel, Eduard: Methods of Conjugate Gradients for Solving Linear Systems. RP 2379, Jour. Res. Nat. Bur. Standards, vol. 49, no. 6, Dec. 1952, pp. 409-436.
3. Turner, L. Richard: Improvement in the Convergence of Methods of Successive Approximation. International Business Machines Corp., 1951. (Reprinted from Proc. Computation Seminar, Dec. 1949.)
4. Glasstone, Samuel, and Edlund, Milton C.: The Elements of Nuclear Reactor Theory. D. Van Nostrand Co., Inc., 1952.